Effect of Amines on Disruption of Cellulose

U.S. DEPARTMENT OF ENERGY
Office of Science

Approach:

- **A complex of cellulose and EDA was used to allow neutron determination of hydrogens.**
- Neutron diffraction was used to analyze the binding and interaction the water and amine hydrogens interacting with cellulose-I.
- EDA (ethylene diamine) can penetrate cellulose fibers.
- MD simulations were used to analyze structures.
- Collaboration between ORNL, Grenoble, and LANL.

Objective:

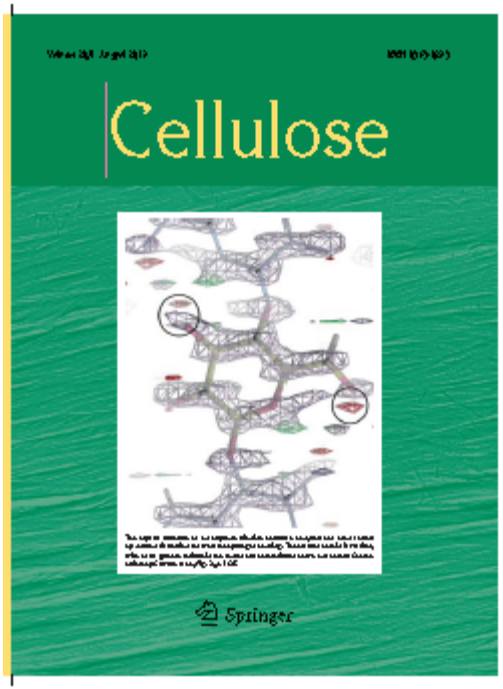
- Use of neutrons and simulations to analyze disruption of cellulose structure.

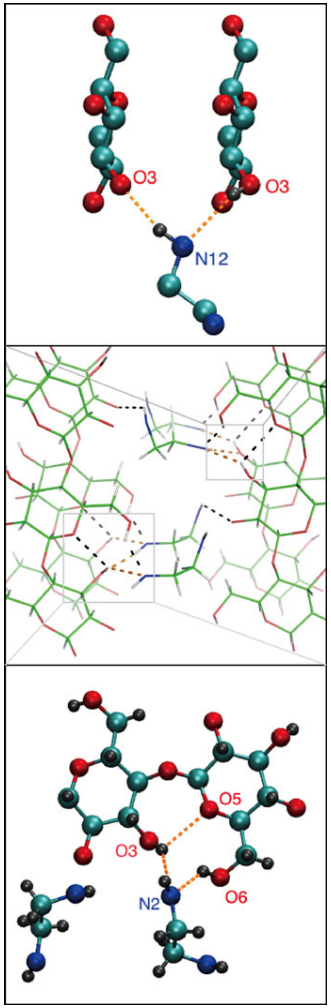
Results:

- There is a cooperative loss of rigidity from the disruption of key oxygen-hydrogen bonds.
- The hydrogen bonding is highly dynamic with bonds being continually being formed and broken thus explaining the difficulty in locating all of the hydrogen atoms in the neutron scattering maps.
- Only about half of the direct H atoms are directly located in the crystal structure.
- *Featured on journal cover.*

Significance:

- Comparison with other polysaccharide-amino complexes supports a common underlying mechanism for amine disruption of cellulose.





Schematic representations of the final neutron structure.

The top and bottom views show projections down the c and a axes with O, C, N and H/D atoms colored red, green, blue and black, respectively, and H-bonds represented by dashed orange lines. The middle view shows the unit cell with the c axis slightly tilted from the vertical direction to show the extended H-bond network.

Citation: D. Sawada, Y. Nishiyama, L. Petridis, R. Parthasarathi, S. Gnanakaran, V. T. Forsyth, M. Wada, P. Langan. "Structure and dynamics of a complex of cellulose with EDA: insights into the action of amines on cellulose". *Cellulose* 20:1563–1571 (2013). Contact: langanpa@ornl.gov

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